Weighted Backprojection Program - *backproj*

Document by James Conway, 10-May-2000. (Incomplete, draft)

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Current version is 1.0.8.

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Overview

The conventions for orientation data (pft) and image data (PIF) formats are the same as those for the current version of ***em3dr*** (Tim Baker, Purdue U.). Typically a selection will be made of the particles refined by ***pft*** and these will be passed to ***em3dr*** or ***backproj*** for reconstruction.

The backprojection may be simple (ie, no weighting), or weighted according to the general geometry procedure of Michael Radermacher. Weighting is strongly recommended, although the run-time will depend the square of the number of images and may become prohibitive for large datasets.

Symmetry may be imposed on the reconstructed density. Icosahedral and several cyclic symmetries are supported.

The ***backproj*** code has been compiled and run on OpenVMS 7.2, Irix 6.5 and Mac OS 8.5 – 9.04. A preliminary version using AltiVec code for PowerPC G4 is almost working.

Input data

Orientations are specified in a pft-format file with either one or two lines of header, followed by orientations. The first line of header contains the input image PIF filename. The second line of header, if it exists, will be ignored.

Images are stored in a single PIF file.

Input parameters can be given interactively, or read from a file.

Output data

The density map is stored in a PIF file. It can be inspected with ROBEM (Rob Ashmore/Tim Baker) or MapView3d (James Conway).

Parameters

1	List of input orientations	`select1.dat`
		`select2.dat`
		`x`

2	Add 90-degrees to omega?	`no`
3	Are origins relative to (1,1) instead of (0,0)	`no`
4	Flip images in Y-axis	`no`
5	Output volume filename	`output.pif`
6	Volume dimensions - cols, rows, slices	`49,49,49`
7	Enter projection mask radius	`25`
8	Enter ray length	`98`
9	Enlargement-factor for the (3D) MAP file	`1.0`
10	Is this Simple, or Weighted back-projection *The data files for projecting may also be used for generating the r-weight function. Alternatively, a different set of files may be used.*	`weighted`
11	Choose same or new	`same`
12	(S)inc function or [M]ixed-Sinc*Gaussian	`mixed`
13	Critical value for Weighting-function (eg, 0.0001)	`0.0001`
14	Pixel size (Angstroms)	`4.2`
15	Center (>8.4)	`30.0`
16	Range (either side of center) *Symmetry can be imposed on the backprojected volume. It may be of the form N22, with 'N'-fold applied around the z-axis and optional 2-folds along the x-axis and/or y-axis, or icosahedral (532) where the 2-fold axes are coincident with the x,y,z-axes. Enter symmetry as follows:* *-- 0 for no symmetry,* *-- N for cyclical z-axis symmetry (eg, 2,3,4,5,6...)* *-- Nxy for cyclical z-axis symmetry with 2-folds on x and/or y axes (eg, 3y,5xy)* *-- 532 for icosahedral symmetry*	`3.0`
17	Symmetry	`532`

Description of Parameters

1	List of input orientations	`select1.dat`
		`select2.dat`
		`x`

Multiple pft-format files are specified here, the list terminating with an 'x'.

2	Add 90-degrees to omega?	`no`
3	Are origins relative to (1,1) instead of (0,0)	`no`
4	Flip images in Y-axis	`no`

These three parameters are mostly obsolete, and will disappear from future version of ***backproj***. For images refined with pft, the answers should typically be "no" to each prompt. For more help with these, please contact James Conway or Eva Kocsis.

5	Output volume filename	`output.pif`

Enter the name of the output file.

6	Volume dimensions - cols, rows, slices	`49,49,49`

Enter the dimensions of the output density map, in pixels.

7	Enter projection mask radius	`25`
8	Enter ray length	`98`

The projection mask radius specifies a radial limit for the input images. Image pixels within this limit will be backprojected. This is a time-saving option which is particularly suited to images of round structures.

Ray length is an equivalent option for the 3d density array, specifying a spherical mask.

In both cases, specify a suitably large mask so as not to truncate density. Units are pixels.

9	Enlargement-factor for the (3D) MAP file	`1.0`

Shrink (<1) or enlarge (>1) the output density. This does not affect the dimensions of the output volume (#6). You should scale these by hand to match any scaling specified here. (Note to myself – check how this affects projection mask radius and ray length).

10	Is this Simple, or Weighted back-projection	`weighted`

"Simple" will run quickly but takes no account of the uneven sampling of orientation space. The result will tend to appear smoother than that from "weighted".

11	Choose same or new	`same`

The data files for projecting may also be used for generating the r-weight function. Alternatively, a different set of files may be used, although this is not often done in practice since it is the distribution of orientations actually used in the reconstruction that should determine the weighting function.

12 (S)inc function or [M]ixed-Sinc*Gaussian `mixed`
The weighting can be modulated by a decaying gaussian, and this is typically what we do.

13 Critical value for Weighting-function (eg, 0.0001) `0.0001`
The magnitude of the weights are limited to this value.

14 Pixel size (Angstroms) `4.2`
Sampling rate of input images. Note that any such parameter in the header of the orientations file(s) is ignored (for now).

15 Center (>8.4) `30.0`
Center of a low-pass filter, in Ångstroms.

16 Range (either side of center) `3.0`
Range of the edge of a low-pass filter, in Ångstroms. A range of 0 specifies a sharp edge. In this example, the onset of the edge is at a spacing of 31.5Å and the filter has decayed to zero at 28.5Å.

17 Symmetry `532`
Symmetry can be imposed on the backprojected volume. It may be of the form N22, with 'N'-fold applied around the z-axis and optional 2-folds along the x-axis and/or y-axis, or icosahedral (532) where the 2-fold axes are coincident with the x,y,z-axes. Enter symmetry as follows:

- 0 for no symmetry,
- N for cyclical z-axis symmetry (eg, 2,3,4,5,6...)
- Nxy for cyclical z-axis symmetry with 2-folds on x and/or y axes (eg, 3y,5xy)
- 532 for icosahedral symmetry

Command line arguments

–a do not use altivec code (PowerPC G4 machines only)
–? display help information
–h display recent history information

Acknowledgements

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